

CURRICULUM VITAE

Personal

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Born: March 8, 1961, West Jefferson, North Carolina USA
Married: June 1, 1991, Angela
Children: Phillip and Zachary

Present Position:

Computational Scientist 236B Wilhelm Hall Scalable Computing Laboratory Ames Laboratory Ames, IA 50011 Phone: (515) 294-9294 Fax: (515) 294-4491 Email: rickyk@ameslab.gov Supervisor: Mark Gordon Start date: Sept. 7 1999	Adjunct Associate Professor Department of Computer Science Iowa State University Ames, IA 50011 Email: rickyk@cs.iastate.edu
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Current Job Duties:

My major function within the Scalable Computing Laboratory at Ames Laboratory is to identify and bring to bear state-of-the-art developments within the field application middleware in such a way as to extend the applicability of high performance computing to computational science and the development of applications from cluster based hardware to high end supercomputers.

I perform this task through a variety of functions:

- by maintaining a watch on the parallel computing industry and gathering performance data on all architectures of interest to the group's activities in computational science.
- by tracking software developments that will enhance portability and reuse of existing and future parallel applications. I have developed, co-developed and use tests that stress all aspects of the underlying hardware - CPU power, disk I/O performance, and communications latency and bandwidth.
- by developing, and collaborating on the development of, a variety of computational algorithms, middleware technologies, languages, and applications on high performance parallel and cluster systems.

Research Interests:

My current research interests cover both the development and implementation of parallel algorithms targeted at high performance computational resources and methods in theoretical and computational chemistry. Furthermore, my computational development activities require the exploitation of these methods across a variety of research areas in computer science and chemical physics. Specifically,

- a. efficient communication sub-system performance and analysis;
- b. mixed mode (process plus threads) algorithmic techniques;
- c. computational resource utilization;
- d. the development of *ab initio* algorithms for parallel systems.
- e. accurate properties of small molecule systems using large basis sets;

Teaching Duties:

- Iowa State University, Department of Computer Science and Department of Electrical and Computer Engineering 425. "High Performance Computing for Scientific and Engineering Applications," Spring 2001-2004.
- Iowa State University, Department of Computer Science 252X, "Linux Operating System Essentials," Summer 2003. This course is now a regular part of the curriculum starting in Fall 2004.

Employment History:

Pacific Northwest National Laboratory, 1989 to 1999.

Staff Scientist
High Performance Computational Chemistry Group
Theory, Modeling, and Simulation Program
Environmental Molecular Sciences Laboratory

Washington State University, Tri-Cities campus, 1995 to 1999.

Adjunct Lecturer,
Electrical Engineering and Computer Science Department.

Education:

Chemistry:

Indiana State University, August 1979 - May 1983, B.S. in Chemistry, Magna Cum Laude.

Attended the University of Utah June 1982 - August 1982 in the Chemistry Department's Undergraduate Research Program working with Professor J. Calvin Giddings.

University of Utah, June 1983 - Oct. 1988, Ph.D. in Chemistry. Research under direction of Professor Jack Simons.

Argonne National Laboratory, Postdoctoral Associate Oct. 1988 - Oct. 1989, Chemistry Division, Research in conjunction with Thom H. Dunning, Jr., and Robert J. Harrison.

Computer Science:

Washington State University, non-degree credit, undergraduate courses in Computer Science 1990-1995.

Object-Oriented Analysis and Design, Richland, WA, December 1993, taught by Advanced Concepts Center, Martin Marietta.

Awards and Fellowships:

Indiana State University Academic scholarship, 1979-1983
Indiana State University Alumni Scholarship, 1979-1983
American Chemical Society Award for Undergraduate Analytical Chemists, 1982
Outstanding Senior Chemistry Student Award, 1983
Member of Phi Kappa Phi, 1983
Indiana State University Dean's List, Fall 1979-Spring 1982, Spring 1983.
University of Utah Entering Graduate Student Scholarship, 1983
Department of Chemistry Research Presentation Award, 1987
Stauffer Graduate Research Prize, 1987
University of Utah Graduate Research Fellowship, 1987-1988
Pacific Northwest National Laboratory,
 Outstanding Team Performance Award, 1996,
 HPCS1 Procurement Team.
Pacific Northwest National Laboratory's FY96 Bonus Program Award
R&D 100 Award for the development of the Molecular Science Software Suite (MS³), 1999.

Memberships in Professional Societies:

Student Affiliate of the American Chemical Society, 1979-1983. Local Chapter President
 at Indiana State University, 1982-1983 academic year.
American Association for the Advancement of Science, 1993-1996.
American Physical Society, 1984-1999.
American Chemical Society, 1989-present.
IEEE Computer Society, 1999-present.

Memberships in High Level National/DOE Committees:

- Executive National Energy Research Scientific Computing Center Users Group (NUGEX) Committee.
- MPP Advisory Council at the National Energy Research Supercomputer Center.

Scientific Publications:

1. P. Acharya, R. Kendall, and J. Simons, "Vibration-Induced Electron Ejection in Molecular Anions", Contributions Symp. At. Surf. Phys., SASP'84, **84**, 1-8 (1984).
2. P. K. Acharya, R. A. Kendall, and J. Simons, "Vibration-Induced Electron Detachment in Molecular Anions", J. Am. Chem. Soc. **106**, 3402-3407 (1984).
3. P. K. Acharya, R. A. Kendall, and J. Simons, "Associative Electron Detachment: O⁻ + H → OH + e⁻", J. Chem. Phys. **83**, 3888-3893 (1985).
4. G. Chalasinski, R. A. Kendall, and J. Simons, "Ab initio Studies of the Structures and Energies of the H⁻(H₂O) and H⁻(H₂O)₂ Complexes", J. Chem. Phys. **87**, 2965-2975 (1987).
5. G. Chalasinski, R. A. Kendall, and J. Simons, "Ab initio Studies of the Structure and Energy of the H⁻(H₂) Complex", J. Phys. Chem. **91**, 6151-6158 (1987).
6. G. Chalasinski, R. A. Kendall, H. Taylor and J. Simons, "Propensity Rules for Vibration-Rotation Induced Electron Detachment of Diatomic Anions: Application to NH⁻ → NH + e⁻", J. Phys. Chem. **92**, 3086-3091 (1988).

7. R. A. Kendall, G. Chalasinski, M. Gutowski, and J. Simons, "The ab initio Energy and Structure of $\text{H}^-(\text{H}_2)_2$ ", *J. Phys. Chem.* **93**, 621-625 (1989).
8. J. A. Nichols, R. A. Kendall, S. Cole, and J. Simons, "Theoretical Study of Anion-Molecule Interactions: $\text{H}^-(\text{HF}) \rightarrow (\text{H}_2)\text{F}^-$ ", *J. Phys. Chem.* **95**, 1074-1076 (1991).
9. R. J. Harrison and R. A. Kendall, "A Parallel Version of ARGOS: A Distributed Memory Model for Shared Memory UNIX Computers", *Theo. Chim. Acta*, **79**, 337-347 (1991)
10. M. M. Szczesniak, R. A. Kendall, and G. Chalasinski, "Ab initio study of the nonadditive effects in the trimer of ammonia", *J. Chem. Phys.* **95**, 5169 (1991).
11. R. A. Kendall, T. H. Dunning, Jr., and R. J. Harrison, "Electron Affinities of the First Row Atoms Revisited", *J. Chem. Phys.* **96**, 6796 (1992).
12. M. W. Feyereisen and R. A. Kendall, "An efficient implementation of the Direct-SCF Algorithm on Parallel Computer Architectures", *Theo. Chim. Acta* **84**, 289 (1993).
13. T. H. Dunning, Jr., S. S. Xantheas, A. C. Hess, D. Feller, R. A. Kendall and R. L. Ornstein "Modeling Molecular Processes in the Environment", Proceedings of the First Energy Research Power Supercomputer Users Symposium, Gaithersburg, Maryland, May 21, 1991, Unrefereed publication.
14. R. A. Bair, M. A. Thompson, R. J. Littlefield, R. A. Kendall, and T. H. Dunning, Jr. "PNL Scientists Gear Up to Solve Environmental Problems", CSCC Update, 13(2), 1992, Unrefereed publication.
15. D. R. Bates, M. F. Guest, and R. A. Kendall, "Enigma of H_3^+ Dissociative Recombination", *Planet. Space Sci.* **41**, 9 (1993).
16. K. A. Peterson, R. A. Kendall, and T. H. Dunning, Jr., "Benchmark Calculations with Correlated Molecular Wave Functions. II. Configuration Interaction Calculations on First Row Diatomic Hydrides", *J. Chem. Phys.* **99**, 1930 (1993).
17. M. W. Feyereisen, R. A. Kendall, J. Nichols, D. Dame, and J. T. Golab, "Implementation of the Direct SCF and RPA Methods on Loosely Coupled Networks of Workstations", *J. Comp. Chem.* **14**, 818 (1993).
18. R. J. Harrison and R. A. Kendall, "Parallel Computing and Chemistry - the vendors and you", *Chemical Design and Automation News*, **8**, 20 (1993).
19. A. P. Rendell, M. F. Guest, and R. A. Kendall, "A Distributed Data Parallel Coupled Cluster Algorithm: Application to the 2-Hydroxypyridine/2-Pyridone Tautomerism", *J. Comp. Chem.* **14**, 1429 (1993).
20. R. A. Kendall "High Performance Computing in Chemistry and Massively Parallel Computers: A Simple Transition?", *Int. J. of Quantum Chem.: Quantum Chem. Symp.* **27**, 769 (1993).
21. K. A. Peterson, R. A. Kendall, and T. H. Dunning, Jr., "Benchmark calculations with correlated molecular wave functions. III. Configuration interaction calculations on first row homonuclear diatomics", *J. Chem. Phys.* **99**, 9790 (1993).
22. D. F. Feller, E. D. Glendening, R. A. Kendall and K. A. Peterson, "An Extended Basis Set Ab Initio Study of $\text{Li}^+(\text{H}_2\text{O})_n$, $n=1-6$.", *J. Chem. Phys.* **100**, 4981 (1994).
23. G. Chalasinski, M. M. Szczesniak, and R. A. Kendall, "Supermolecular approach to many-body dispersion interactions in weak van der Waals complexes: He, Ne, and Ar trimers", *J. Chem. Phys.* **101**, 8860 (1994).
24. R. A. Kendall and M. F. Guest, "Input and Output in Chemistry Applications", in *Grand Challenges in Computer Simulation, High Performance Computing 1995*, Proceedings of the 1995 Simulation Multiconference, Ed. A. M. Tentner, Society for Computer Simulation (1995), pp, 522-526.

25. M. F. Guest, E. Apra, D. E. Bernholdt, H. A. Frücht, R. J. Harrison, R. A. Kendall, R. A. Kutteh, J. B. Nicholas, J. A. Nichols, M. S. Stave, A. T. Wong, R. J. Littlefield and J. Nieplocha, "High Performance Computational Chemistry; Towards Fully Distributed Parallel Algorithms", in Grand Challenges in Computer Simulation, High Performance Computing 1995, Proceedings of the 1995 Simulation Multiconference, Ed. A. M. Tentner, Society for Computer Simulation (1995), pp. 511-521.
26. R. A. Kendall, R. J. Harrison, R. J. Littlefield, and M. F. Guest, "High Performance Computational Chemistry: Methods and Machines", chapter 4, pp. 209-316, in "Reviews in Computational Chemistry, Volume VI", Eds. K. B. Lipkowitz and D. B. Boyd, VCH Publishers, Inc., New York (1995).
27. D. F. Feller, R. A. Kendall, and M. J. Brightman, "The EMSL Ab Initio Methods Benchmark Report: A Measure of Hardware and Software Performance in the Area of Electronic Structure Methods, Version 2", PNNL Technical Report., Unrefereed publication. (1995).
28. M. F. Guest, R. A. Kendall, J. A. Nichols., T. H. Dunning, Jr., and M. S. Gordon, Editors, "Opportunities and Challenges of High Performance Computing in Chemistry", Workshop report from the High Performance Computational Chemistry workshop, Bethesda, March 1993. PNNL Technical Report., Unrefereed publication. (1995).
29. D. E. Bernholdt, E. Apra, H. A. Frücht, M. F. Guest, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, J. Nieplocha, "Parallel Computational Chemistry Made Easier: The Development of NWChem", Int. J. Quantum Chem. Symp. **29**, 475, (1995).
30. M. F. Guest, E. Apra, D. E. Bernholdt, H. A. Frücht, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha, "High performance computational chemistry: NWChem and fully distributed parallel application," pp. 278-294, in "Applied Parallel Computing. Computation in Physics, Chemistry and Engineering Science. Second International Workshop, PARA '95. Proceedings," Eds. J. Dongarra, K. Madsen, J. Wasniewski, Springer-Verlag, Berlin, Germany 1996. Conference: Lyngby, Denmark, 21-24 Aug 1995.
31. M. F. Guest, E. Apra, D. E. Bernholdt, H. A. Frücht, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield and J. Nieplocha, "High Performance Computational Chemistry: NWChem and Fully Distributed Parallel Applications", in Advances in Parallel Computing, 10, High Performance Computing: Technology, Methods, and Applications, Eds. J. Dongarra, L. Gradietti, G. Joubert, and J. Kowalik, (Elsevier Science B. V. pp. 395-427, 1995).
32. I. T. Foster, J. L. Tilson, A. F. Wagner, R. Shepard, R. J. Harrison, R. A. Kendall, and R. J. Littlefield, "Toward High-Performance Computational Chemistry: I. Scalable Fock Matrix Construction Algorithms", J. Comput. Chem., **17**, 109, 1996.
33. R. J. Harrison, M. F. Guest, R. A. Kendall, D. E. Bernholdt, A. T. Wong, M. Stave, J. L. Anchell, A. C. Hess, R. J. Littlefield, G. I. Fann, J. Nieplocha, G. S. Thomas, D. Elwood, J. Tilson, R. L. Shepard, A. F. Wagner, I. T. Foster, E. Lusk and R. Stevens, "Toward High-Performance Computational Chemistry: II. A Scalable Self Consistent Field Program", J. Comput. Chem., **17**, 124, (1996).
34. M. F. Guest, E. Apra, D. E. Bernholdt, H. A. Frücht, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield, and J. Nieplocha, "High-performance Computing in Chemistry; NWChem," Future Generation Computer Systems, **12**, 273, (1996). PNL-SA-27337.
35. S. M. Cybulski, R. A. Kendall, G. Chalasinski, M. W. Severson, and M. M. Szczesniak, "Ab initio study of the O₂(X ³ Σ_g^-) + Ar(¹S) van der Waals interaction," J. Chem. Phys. **106**, 7731, (1997).
36. H. A. Frücht, R. A. Kendall, R. J. Harrison and K. G. Dyall, "A Parallel Implementation of RI-SCF on Parallel Computers", Int. J. Quant. Chem. **64**, 63, (1997).
37. D. Feller, M. A. Thompson, and R. A. Kendall, "A Theoretical Case Study of Substituent Effects on the Binding Specificity of Crown Ethers" J. Phys. Chem. A. **101**, 7292 (1997).

38. R. A. Kendall, and H. A. Früchtl, “The impact of the Resolution of the Identity (RI) approximate integral method on modern *ab initio* algorithm development”, *Theoretical Chemistry Accounts* **97**, 158 (1997).
39. R. D. Hasse, M. W. Severson, M. M. Szczesniak, G. Chalasinski, P. Cieplak, R. A. Kendall, and S. M. Cybulski, “Ar-C₂H₂: A challenging system for *ab initio* calculations,” *J. Molecular Structure* **436-437**, 387-400, (1997).
40. R. A. Kendall, G. Chalasinski, J. Klos, R. Bukowski, M. W. Severson, M. M. Szczesniak, and S. M. Cybulski, “Ab initio study of van der Waals interaction of NH(X ³ Σ^-) with Ar(¹S)” *J. Chem. Phys.* **108**, 3235 (1998).
41. I. Foster, J. Nieplocha, and R. A. Kendall “ChemIO: High-Performance Parallel I/O for Computational Chemistry Applications,” *The International Journal of High Performance Computing Applications*, **12**, 345-363, (1998).
42. J. L. Tilson, M. Minkoff, A. F. Wagner, R. Shepard, P. Sutton, R. J. Harrison, R. A. Kendall, and A. T. Wong, “High Performance Computational Chemistry: Hartree-Fock Electronic Structure Calculations on Massively Parallel processors,” *International Journal of High Performance Computing Applications*, **13**(4), 291-302 (1999).
43. R. A. Kendall, E. Aprà, D. E. Bernholdt, E. J. Bylaska, M. Dupuis, G. I. Fann, R. J. Harrison, J. Ju, J. A. Nichols, J. Nieplocha, T. P. Straatsma, T. L. Windus, and A. T. Wong, “High Performance Computational Chemistry; an Overview of NWChem a Distributed Parallel Application” *Computer Physics Communications*, **128**, 260-283 (2000).
44. B. Bode, D. M. Halstead, R. Kendall, Z. Lei, and D. Jackson, “The Portable Batch Scheduler and the Maui Scheduler on Linux Clusters”, Proceedings from the 4th Annual USENIX Extreme Linux Conference, pp. 217-224 (2000).
45. K. Parzyszek, J. Nieplocha and R. A. Kendall, “A Generalized Portable SHMEM Library for High Performance Computing”, Proceedings of the IASTED Parallel and Distributed Computing and Systems 2000, Las Vegas, Nevada, November 2000, (M. Guizani and X. Shen, Eds.), pp. 401-406. IASTED, Calgary (2000).
46. Y. Alexeev, R. A. Kendall, and Mark S. Gordon, “The Distributed Data SCF,” *Computer Physics Communications*, **143**, 69-82, (2002).
47. D. Turner, W. Chen, and R. Kendall, “Performance of the MP_Lite message-passing library on Linux cluster”, Proceedings of Linux Clusters: The HPC Revolution, June 25-27, 2001, NCSA, Urbana, IL (2001).
48. M.-S. Wu, S. Aluru, and R. A. Kendall, “Mixed Mode Matrix Multiplication,” in Proceedings of the IEEE International Conference on Cluster Computing, Cluster 2002, Chicago, IL, September 24-26, 2002, pp. 195-203, IEEE Computer Society, Los Alamitos, CA, (2002).
49. Y. Alexeev, M. Schmidt, T. Windus, M. S. Gordon, and R. A. Kendall, “Performance and implementation of Distributed Data CPHF and SCF algorithms,” in Proceedings of the IEEE International Conference on Cluster Computing, Cluster 2002, Chicago, IL, September 24-26, 2002, pp. 135-141, IEEE Computer Society, Los Alamitos, CA, (2002).
50. Z. Gan, Y. Alexeev, R. A. Kendall, and Mark S. Gordon, “A Distributed Data Implementation of Parallel Full CI Program,” in Proceedings of the IEEE International Conference on Cluster Computing, Cluster 2002, Chicago, IL, September 24-26, 2002, pp. 476-479, IEEE Computer Society, Los Alamitos, CA, (2002).
51. K. Parzyszek and R. A. Kendall, “GPSHMEM: application to kernel benchmarks,” in the Proceedings of the Fourteenth IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2002) Cambridge, MA, November 4-6, 2002, pp. 404-409. ACTA Press, Anaheim, CA. (2002).
52. Z. Gan, Y. Alexeev, M. S. Gordon, and R. A. Kendall, “The parallel implementation of a full configuration interaction program,” *J. Chem. Phys.* **119**, 47-59, (2003).
53. L. Huang, B. Chapman, R. Kendall, “OpenMP for Clusters,” Proceedings of Fifth European Workshop on OpenMP, Aachen, Germany September 22-23, 2003.

54. L. Huang, B. Chapman, R. Kendall, "OpenMP on Distributed Memory via Global Arrays," Proceedings of Parallel Computing 2003 (ParCo2003), Dresden, Germany, September 2-5, 2003.
55. M.-S. Wu, R. A. Kendall, S. Aluru, "A Tunable Collective Communication Framework on Cluster of SMPs," Proceedings of the IASTED International Conference on Parallel and Distributed Computing and Networks (PDCN 2004), Innsbruck, Austria, February 17-19, pp. 56-63 2004.
56. J. Bentz and R. A. Kendall, "Parallelization of general matrix multiply routines using OpenMP," in the Proceedings of the Workshop on OpenMP Applications and Tools, WOMPAT 2004, Houston, TX, May 17-18, 2004.
57. M.S. Wu, R. A. Kendall, and S. Aluru, "Exploring Collective Communications on a Cluster of SMPs," in the Proceedings of 7th International Conference on High Performance Computing and Grid in Asia Pacific Region, HPCAsia2004, Omiya Sonic City, Tokyo Area, Japan, July 20-22, pp. 114-117, 2004.
58. Submitted papers:
 - J. Bentz and R. A. Kendall, "Parallelization of general matrix multiply routines using OpenMP," submitted to Lecture Notes in Computer Science.

Scientific Software:

- J. A. Nichols, M. R. Hoffmann, R. A. Kendall, H. L. Taylor, D. W. O'Neal, E. Earl, R. Hernandez, M. Gutowski, X. Wang, J. Rusho, J. Boatz, J. L. Anchell, K. Bak, and J. Simons, 1986 - 1994. Utah Messkit: Molecular integrals and integral derivatives, Direct CI, Davidson-Liu Diagonalization, Non-Born Oppenheimer matrix elements.
- R. A. Kendall, Maintenance and ports of Columbus, Sirius and Messkit to Harris, Multiflow, FPS 164, Vax8200 for Simons Group. 1984-1988.
- R. J. Harrison and R. A. Kendall, PARGOS: MIMD parallel version of COLUMBUS integral program, 1989.
- R. A. Kendall, Utah Messkit, Shared memory and MIMD replicated-data parallel version of conventional SCF, 1989, 1992.
- R. J. Harrison and R. A. Kendall, Selected CI with RS MP2 Perturbative Estimates. Parallel version on work-station clusters, Intel Delta, Intel iPSC860, 1992, 1993.
- M. W. Feyereisen, R. A. Kendall, J. Almlöf, J. A. Nichols, D. Dame and J. T. Golab, Replicated Data Parallel DISCO. SCF, gradients, and RPA, 1991-1993.
- Anchell, J.; Apra, E.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dupuis, M.; Dyall, K.; Fann, G.; Fruchtl, H.; Gutowski, M.; Harrison, R.; Hess, A.; Jaffe, J.; Kendall, R.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nichols, J.; Nieplocha, J.; Rendall, A.; Stave, M.; Straatsma, T.; Taylor, H.; Thomas, G.; Wolinski, K.; Wong, A.; "NWChem, A Computational Chemistry Package for Parallel Computers, Version 3.0" (1997), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA. I develop and coordinate developments primarily for the Integral API, McMurchie-Davidson integrals and gradients, of third party integral codes, Basis Set Object, ECP API, RI SCF, QM/MM, and geometry optimization software, 1993-2001.
- Krzysztof Parzyszek, Jarek Nieplocha, and Ricky A. Kendall GPSHMEM, "A Generalized Portable SHMEM implementation", 2000-2001.

Workshops organized or co-organized:

- “High Performance Computational Chemistry” (NIH, Bethesda, March 1993), funded by the National Science Foundation, Argonne National Laboratory, the Office of Scientific Computing, the Division of Chemical Sciences, Office of Basic Energy Sciences and the Environmental Management Office of the U.S. Department of Energy, and the National Institutes of Health.
- “High Performance Computational Chemistry Workshop” (Pleasanton Hilton, Pleasanton, CA, August 1995), funded by the Office of Mathematical, Information and Computational Sciences, the Environmental Molecular Sciences Laboratory Project of the Office of Environmental Management in the Office of Energy Research of the U.S. Department of Energy, the National Energy Research Supercomputer Center and the National Institutes of Health.
- “West Coast Theoretical Chemistry Conference 1998”, (PNNL, Richland, WA June 1998)
- “IEEE International Conference on Cluster Computing, Cluster 2002, Chicago, IL, September 24-26, 2002,” Poster Chair.
- 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, IA, June 12-14, 2003. Co-Organizer.
- Workshop on OpenMP Applications and Tools, University of Houston, Houston, Texas, May, 2004. Program Committee.

Invited Presentations and Contributions:

Presentations:

- “The Molecular Science Research Center and the Environmental and Molecular Sciences Laboratory at Pacific Northwest Laboratory”, Indiana State University Chemistry Department, Terre Haute, Indiana, August 1990.
- Lecturer at the School for Parallel Computing in Theoretical Chemistry and Physics at the University of Vienna, Vienna, Austria, September 1991.
- “High Performance Computational Chemistry at Pacific Northwest Laboratory”, National Institutes of Health, Division of Computer Research and Technology, Bethesda, Maryland, May 1992.
- “Does High Performance Computing Change the Way in Which We Do Computational Chemistry?”, Panel Discussion for Supercomputing 92, Minneapolis Minnesota, November 1992.
- “High Performance Computing in Chemistry and Massively Parallel Computers: A Simple Transition?”, Sanibel Symposium 1993, Session on Advanced Scientific Computing - Methods, Algorithms, Tools, and Architectures, St. Augusting, Florida, March 1993.
- “Current MPP Vendor Offerings and the Computing Environment”, University of Utah Faculty Computing Advisory Group, Salt Lake City, Utah, April 1993.
- “Input and Output in Chemistry Applications”, Grand Challenges in Computer Simulation, High Performance Computing 1994, Simulation Multiconference, sponsored by the Society for Computer Simulation, San Diego, California, April 1994
- “Computational Chemistry Application Design for Massively Parallel Supercomputers”, Gordon Conference on Computational Chemistry, Session on Massively Parallel Computing and Applications, New Hampton, New Hampshire, July 1994.
- “Parallel Computing and Computational Chemistry: the NWChem Story”, the National Energy Research Supercomputer Center Massively Parallel Processing Workshop, NERSC, Lawrence Livermore National Laboratory, Livermore, California, June 14th, 1995.

- “Parallel Computing and Computational Chemistry: the NWChem Software Suite”, Parallel Infrastructures for Applications Workshop, University of Texas, Austin, Texas 78712, April, 1996
- “The double edged sword of high performance computational chemistry development: One Developer’s Perspective”, Mardi Gras Conference ’97, Multiscale Phenomena in Science and Engineering, Louisiana State University, Baton Rouge, Louisiana, February 7-9, 1997.
- “NWChem, High Performance Computational Chemistry Software; the need and the implementation”, Department of Chemistry and Biochemistry, Oakland University, Rochester, Michigan, January 1998.
- “NWChem, High Performance Computational Chemistry Software; the need and the implementation”, Department of Chemistry, Indiana State University, Terre Haute, Indiana, January 1998.
- “Anyone ever hear of the Manhattan Project?”, Turkey Run High School, Turkey Run, Indiana, January 1998.
- “NWChem, High Performance Computational Chemistry Software; the functionality and usability,” Department of Chemistry, Indiana University Purdue University at Indianapolis, Indianapolis, Indiana, May 1999.
- “Scalable Computing Laboratory and Programming Models,” Department of Computer Science, University of Northern Iowa, Cedar Falls, Iowa, April 2002.
- “Where are programming models going and what is the impact on application development?” Eleventh SIAM Conference on Parallel Processing for Scientific Computing (PP04), San Francisco, California, February 25-27, 2004.

Contributions:

- Tutorials Committee, The International Conference for High Performance Networking and Computing, SC2004, Pittsburgh, Pennsylvania. Nov 2004.
- Tutorials Committee, The International Conference for High Performance Networking and Computing, SC2003, Phoenix, Arizona. Nov 2003.
- Technical Papers Committee, The International Conference for High Performance Networking and Computing, SC2002, Baltimore, Maryland. Nov 2002.
- Technical Papers Committee, The International Conference for High Performance Computing and Communications, SC2000, Dallas, Texas. Nov 2000.
- Member of the MPP Advisory Council at NERSC (the National Energy Research Scientific Computer Center). As the sole PNNL representative, I provide input on MPP specifications, goals, and products.
- Member of the Executive Energy Research Supercomputer Users Group (ExERSUG) Committee. As the Chemical Sciences, Office of Basic Energy Sciences representative, I provide input to the NERSC management on utilization, purchase, and allocation of resources for the 3000+ user community. I am currently the Chair of ExERSUG, (Jan 1996 - April 1998), and was the Vice-chair for one year, (Jan 1995 - Jan 1996)
- I was a member of the EMSL Source Evaluation Panel for the purchase of High Performance Computing Systems. This involved the specification of requirements, analysis of vendor offerings, and acceptance of the delivered systems, a two year process. The first effort, for HPCS-0, delivered 80 node KSR2 in 1993. The second procurement ultimately delivered a 512 node IBM-SP supercomputer.
- Scalable I/O (SIO) Initiative:

The SIO Initiative is a multi-institutional (20+ sites in the Concurrent Supercomputer Consortium) collaboration supported by multiple funding agencies (ARPA, NSF, NASA, DOE) targeted at developing the enabling technology to produce a scalable I/O subsystem for MPP supercomputers. This includes Operating Systems, Language Library, Hardware, Compiler, Performance Measurement, and Application researchers.

- Technical Steering Committee: I represent the Applications Working Group on the steering committee that provides guidance to the six main working groups of the Initiative.
- Applications Working Group: I was the co-chair of the group responsible for designing, testing, and tracking applications and applications templates that stress and measure the performance of the scalable I/O subsystem being developed under the SIO initiative.

Postdoctoral and Student researchers:

Graduate Student: Dr. Krzysztof Parzyszek (Jan. 2000 to Jul 2003)

Department: Computer Science @ Iowa State University

Project: Genralized Portable SHMEM Library

Current Position: IBM Compiler Group, Toronto Canada

Graduate Student: Weiye Chen (Summer 2000 to Summer 2001)

Department: Computer Science @ Iowa State University

Project: OS Bypass Modules for MP_Lite & Compression Library

Graduate Student: Meng-Shiou Wu (Fall 2000 to present)

Department: Computer Engineering @ Iowa State University

Project: Mixed Programming Models for Matrix Multiply and Cache Aware/Oblivious Algorithms

Student: Douglas J. Fuller (2000 to 2002.)

Department of Computer Science

Iowa State University, Ames, IA.

Project: Distributed Shared Memory Translation Tool

Student: Danille Farrar (Aug. 1997 to Aug 1998.)

Inquiring Into Science Program

Richland High School, Richland WA

Project: Java Programming of the NWChem support tool and a personal Queueing system.

Postdoctoral Appointee: Dr. Zhengting Gan (2002-2003)

Project: "Algorithms in Parallel Full Configuration Interaction:

Computational Chemistry:"

Current Position: Postdoctoral Fellow, Oak Ridge National Laboratory

Postdoctoral Appointee: Dr. Herbert A. Früchtl (1993-1997)

Erlangen University, Germany

Project: "Algorithms in MPP Computational Chemistry:

Implementation and Applications"

- Scalable Gradient Technology;

- Scalable RI-SCF implementation;

- RI-SCF gradient approximations;

- Van der Waals Complexes, Ar-N₂O;

- Frequency analysis of large systems;

Student: Pawel Wolinski (Dec. 1995 to May 1996, Summer 1997)

Computer Science Dept.

University of Arkansas

Project: WWW documentation procedures for HPCCG (1995/6)

Python integration in NWChem (with RJ Harrison)

Student: Matthew J. Brightman (Summer, 1994, 1995)

Project: Kennewick High School
The Performance of parallel GAMESS-US (1994)
Automation of WWW documentation for HPCCG (1995)

Student: Mary E. Powers (1992-1993)
Washington State University
Computer Science Dept.

Project: XRCS a graphical interface to the RCS revision control system.

References

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